

Geant4-related R&D for new particle transport methods

M. Augelli, M. Begalli, T. Evans, E. Gargioni, S. Hauf, C. H. Kim, M. Kuster, M. G. Pia, P. Queiroz Filho, L. Quintieri, P. Saracco, D. Souza Santos, G. Weidenspointner, A. Zoglauer

Abstract—A R&D project has been launched in 2009 to address fundamental methods in radiation transport simulation and revisit Geant4 kernel design to cope with new experimental requirements. The project focuses on simulation at different scales in the same experimental environment: this set of problems requires new methods across the current boundaries of condensed-random-walk and discrete transport schemes. An exploration is also foreseen about exploiting and extending already existing Geant4 features to apply Monte Carlo and deterministic transport methods in the same simulation environment. An overview of this new R&D associated with Geant4 is presented, together with the first developments in progress.

I. INTRODUCTION

GEANT4 [1], [2] is an object oriented toolkit for the simulation of particle interactions with matter. It provides advanced functionality for all the domains typical of detector simulation: geometry and material modelling, description of particle properties, physics processes, tracking, event and run management, user interface and visualisation.

Geant4 is nowadays a mature Monte Carlo system; its multidisciplinary nature and its wide usage are demonstrated by the fact that its reference article [1] is the most cited publication [3], [4] in the Nuclear Science and Technology category.

Geant4 is the result of a R&D project (CERN RD44) [5] carried out between 1994 and 1998. RD44 was launched at a time when the LEP experiments were running GEANT 3 as a well-established system, that had been refined throughout a decade of production service. RD44 investigated the adoption of the object oriented technology and C++ for a simulation

system replacing GEANT 3.21 [6], and developed the first functional version of the Geant4 released at the end of 1998.

The Geant4 releases following the first Geant4 one at the end of 1998 have added new functionality to the toolkit; nevertheless, its architectural design and the fundamental concepts of Geant4 application domain have remained substantially unchanged since their original conception.

New experimental requirements have emerged in the recent years, which challenge the conventional scope of major Monte Carlo transport codes like Geant4. Research in nanodosimetry, nanotechnology-based detectors, radiation effects on components in space and at high luminosity colliders, nuclear power, plasma physics etc. have shown the need of new methodological approaches to radiation transport simulation along with new physics functionality in Geant4. A common requirement has emerged in all such research domains, i.e. the ability to change the scale at which the problem is treated in a complex simulation environment. This requirement goes beyond the traditional issues of variance reduction, for which current Monte Carlo codes provide abundant tools and techniques.

Significant technological developments both in software and computing hardware have also occurred since the RD44 phase. New software techniques are available nowadays, that were not yet established at the time when Geant4 was designed.

II. RECENT EXPERIMENTAL EVOLUTIONS AND REQUIREMENTS

Various experimental domains would profit of the capability of dealing with co-working transport schemes.

Radiation effects at the nano-scale are important for the protection of electronic devices operating in various radiation environments. In realistic use cases small-scale systems are often embedded in larger scale ones: for instance, a component may operate within a collider experiment or on a satellite in space, cellular and sub-cellular aggregates in real biological systems exist in complex body structures etc. A simulation system capable of addressing different scales would be relevant to studies of the effects on components exposed to the fierce experimental environment of LHC (and future super-LHC).

The capability of condensed and discrete Monte Carlo simulation schemes in the same software environment is also critical to experimental configurations involving nanotechnology-based detectors. While R&D in nanotechnology is actively pursued also in view of application to HEP detectors, it is not yet possible to simulate such detectors as standalone systems with Geant4, nor to evaluate their performance once they are embedded in a full-scale experimental set-up.

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Mauro Augelli is with the Centre d'Etudes Spatiales (CNES), Toulouse, France.

Marcia Begalli is with State University of Rio de Janeiro, Brazil.

Thomas Evans is with Oak Ridge National Laboratory, Oak Ridge, TN, USA.

Elisabetta Gargioni is with University Medical Center Hamburg-Eppendorf, Germany.

Steffen Hauf and Markus Kuster are with University of Technology, Darmstadt, Germany.

Chan Hyeong Kim is with Hanyang University, Seoul, Korea.

Maria Grazia Pia and Paolo Saracco are with INFN Sezione di Genova, Via Dodecaneso 33, 16146 Genova, Italy (e-mail: MariaGrazia.Pia@ge.infn.it, Paolo.Saracco@ge.infn.it).

Pedro Queiroz Filho and Denison Souza Santos are with Institute for Radiation Protection and Dosimetry IRD, Rio de Janeiro, Brazil.

Lina Quintieri is with INFN Laboratori Nazionali di Frascati, Frascati, Italy.

Georg Weidenspointner is with the Max-Planck-Institut für extraterrestrische Physik, Postfach 1603, 85740 Garching, Germany, and with the MPI Halbleiterlabor.

Andreas Zoglauer is with the Space Sciences Laboratory, University of California at Berkeley, Berkeley, CA, USA.

Plasma physics requires addressing the concept of object state and behaviour mutation in relation to the environment: in this use case the mutability concerns both the physics processes and the particles involved. Astrophysics and studies for fusion-based nuclear power are just two relevant applications, which would profit of Geant4 applicability to this physics domain.

The issue of co-existing condensed-random-walk and discrete schemes arises in another context of the simulation domain. It concerns the conceptually correct treatment of the atomic relaxation following the impact ionization produced by charged particles: since the cross section for producing secondary electrons from ionization is subject to infrared divergence, in the conventional condensed-random-walk schemes the interaction is treated in two different regimes of continuous energy loss along the step and of discrete X-ray production, with the consequent adoption of cutoffs. This scheme introduces an artificial dependency on cuts in the generation of PIXE (Particle Induced X-ray Emission), while atomic relaxation is intrinsically a discrete process; moreover, the current Geant4 scheme neglects the correlation between the X-ray spectrum of primary ionization and PIXE. A conceptual revision of the continuous energy loss and discrete scheme would be desirable in this physics domain too. Use cases affected by the current conceptual limitation to treat PIXE correctly in Geant4 involve multiple, multi-disciplinary domains: applications for material analysis from planetary science to cultural heritage, precise dosimetry, critical shielding optimization of X-ray telescopes etc.

III. MAIN AREAS OF RESEARCH

A R&D project, named NANO5, has been recently launched [7] to address fundamental methods in radiation transport simulation; it explores possible solutions to cope with the new experimental requirements mentioned in the previous section and evaluates whether and how they can be supported by Geant4 kernel design. It was initiated by a team at the Italian Institute of Nuclear Research (INFN) and currently gathers an international team of physicists and engineers with background in various disciplines.

The main focus of the project lies in the simulation at different scales in the same experimental environment: this objective is associated with the research of transport methods across the current boundaries of condensed-random-walk and discrete transport schemes. An exploration is also foreseen about exploiting and extending already existing Geant4 features to apply Monte Carlo and deterministic transport methods in the same simulation environment. The Geant4 toolkit is the ideal playground for this research, thanks to the object oriented technology it adopted in the RD44 phase.

Other issues have been identified along with the experience of Geant4 development and usage over the past 10 years, which would profit of the exploratory research in the kernel design motivated by the main objectives of the project:

- Customization of physics modeling in a simulation application
- Scattered and tangled concerns across the code

- Facilities for physics verification and validation
- Performance

These topics are considered as supporting developments, which are instrumental to achieve the main goals of the project.

The project adopts a software process model based on the Unified Process [8] framework. The software developments are motivated by concrete experimental applications, and significant effort is invested in the software design: these features of the project are well served by the Unified Process, which is use case driven and architecture-centric. The adopted software process framework involves an iterative and incremental life-cycle.

IV. CO-WORKING CONDENSED AND DISCRETE SIMULATION METHODS

Methods to model hard interactions of particles with matter constituents by means of an appropriate binary theory are well established: in this approach collisions are treated as binary processes, that is, either the target electrons are treated as free and at rest, or the influence of binding is accounted only in an approximated way.

General-purpose Monte Carlo codes, like EGS [9], [10], [11], FLUKA [12], [13], Geant4 and MCNP [14], [15], [16], operate in this context. Their calculations of energy deposit distributions are based on condensed-random-walk schemes of particle transport. Charged particle tracks are divided into many steps, such that several interactions occur in a step; one energy loss and one deflection are calculated for each step. A further simplification consists in the adoption of the Continuous Slowing Down Approximation (CSDA), where the energy loss rate is determined by the stopping power. This approach is adequate as long as the discrete energy loss events treated are of magnitudes larger than electronic binding energies.

Various specialized Monte Carlo codes, usually known as “track structure codes”, have been developed for micro and nano-dosimetry calculations. They handle particle interactions with matter as discrete processes: all collisions are explicitly simulated as single-scattering interactions. This approach is suitable to studies where the precise structure of the energy deposit and of the secondary particle production associated with a track is essential; nevertheless, the detailed treatment of collisions down to very low energy results in a high computational demand.

So far, simulation based on condensed-random-walk schemes and so-called track structure generation have been treated as distinct computational domains; this separation is due to the conceptual and technical difficulty of handling the two schemes in the same simulation environment. Achieving a conceptual approach and an architectural design where the two schemes can co-work would represent a significant progress in Monte Carlo simulation.

Recently, a set of specialized processes for track structure simulation in liquid water has been designed and implemented in Geant4 [19]; like their equivalents in dedicated Monte Carlo codes, they operate in the regime of discrete interactions. While the toolkit nature of Geant4 allows the co-existence of

tools for simulation at different scales, the capability of these two schemes to effectively co-work in a multi-scale problem is still far from being established.

V. CO-WORKING MONTE CARLO AND DETERMINISTIC SIMULATION METHODS

Deterministic transport methods are widely used in various domains: radiotherapy treatment planning and calculations for nuclear reactors are just two examples. Their usage is motivated by the requirement of a fast simulation response in complex situations.

Both Monte Carlo and deterministic transport methods have their own strong points and limitations. Research in this field to perform both transport models within the same simulation environment would be highly valuable: the capability of different transport methods in the same simulation environment would simplify the geometrical and material modelling of the system under study, and would facilitate the analysis of the behaviour of the system itself.

VI. SUPPORTING RESEARCH TOPICS

The complexity of the problem domain to be addressed requires the investigation of software techniques, capable to effectively support the conceptual objectives to be pursued.

A. Generic programming techniques in physics simulation design

Metaprogramming has emerged in the last few years as a powerful software technique. In C++ the template mechanism provides naturally a rich facility for metaprogramming; libraries like Boost [17] and Loki [18] are nowadays available to support generic programming development. Metaprogramming presents several interesting advantages, which propose it as a worthy candidate for physics simulation design.

This technique has not been exploited in Geant4 core yet: the evolution towards the C++ standard still in progress and the limited support available in C++ compilers at the time of the RD44 phase discouraged the consideration of templates for extensive use in Geant4 architectural design at that stage.

A preliminary investigation of its applicability in a multi-platform simulation context has been carried out by one of the authors of this paper through the application of a policy-based class design [19] limited to a restricted physics sub-domain.

B. Design for scattered and tangled concerns

The problem domain of radiation transport simulation involves a number of concerns, which are common to multiple parts of the system, but whose code gets scattered across different parts; moreover, multiple concerns may be tangled in the same code. The capability of addressing scattered concerns by an effective design would result in leaner, more easily maintainable code: an optimization in this domain would be meaningful in a large-scale software system like Geant4.

The object oriented technology lacks proper instruments to address the issue of scattering and tangling of concerns.

Aspect oriented programming provides support for cross-cutting concerns (i.e. aspects) and for automatically propagating appropriate points of execution in the code; nevertheless, this technology is not widely established yet, and language support is still relatively limited in C++.

Two topics associated to concerns in Geant4 code are relevant to the research areas considered in this project: the issue of endowing objects - in particular, physics objects - of intrinsic verification and validation capabilities (more in general, of analysis capabilities), and dealing with secondary effects following a primary interaction (e.g. the relaxation of an excited atom). An exploratory study in these areas would be useful to evaluate the possibility of addressing concerns effectively in a simulation environment like Geant4.

VII. ONGOING ACTIVITIES

The activity currently in progress has an exploratory character: it evaluates various problem domains to identify the issues to be addressed, the requirements in the associated experimental domains and candidate technologies.

Regarding the main topic of research, the problem domain analysis has identified the concept of “mutability” as a main issue in the context of transition between co-working condensed and discrete transport schemes. The current research in software design explores the introduction of the concept of “mutants” in the software design, and of “stimuli” capable of triggering mutations. Related concepts, like reversible and spontaneous mutation, are subject to investigation too.

The introduction of the concept of mutability in physics-related objects requires the identification of their stable and mutable states and behaviour, and their fine-grained decomposition into parts capable of evolving, or remaining unchanged. Two pilot projects are in progress to explore the capability of policy-based class design to support this requirement in two large scale physics simulation domains: a general-purpose one [20] and a “track structure” one.

Issues related to PIXE simulation are explored in another dedicated pilot project [21], [22].

In parallel, a project focussed on the simulation of radioactive decay [23] explores issues related to the collaboration between electromagnetic and hadronic components of the design associated with the prototypes explored in the electromagnetic domain.

VIII. CONCLUSION AND OUTLOOK

A R&D project is in progress to address the capability of dealing with multi-scale use cases in the same simulation environment based on Geant4: this requirement involves the capability of handling physics processes according to different transport schemes. The first developments associated with this project are described in greater detail in other contributions to the 2009 IEEE Nuclear Science Symposium Conference Record. M. Kuster and S. Hauf acknowledge support by the Bundesministerium für Wirtschaft und Technologie and the Deutsches Zentrum für Luft- und Raumfahrt - DLR under the grant number 50QR0902.

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